The inverse tangent algorithm used by the KDF9

Introduction

The interdependent sequences $\{a_i\}$ and $\{b_i\}$ generated by the recurrence relations

$$a_{i+1} = \frac{1}{2}(a_i + b_i) \tag{1}$$

and

$$b_{i+1} = \sqrt{a_{i+1} b_i}, \tag{2}$$

from starting values $\{a_0\} = 1$ and $\{b_0\} = \sqrt{1+x^2}$, form the basis of the algorithm used by the KDF9 to calculate the inverse tangent of x. We derive the algorithm below. At first glance the sequences seem to come 'out of the blue'; we provide some motivation for their use below.

The Algorithm

Let $x = \tan\theta$. The members of sequence $\{a_i\}$ satisfy

$$a_i = 2^{-i} x \cot\left(2^{-i} \mathrm{arctan} x\right), \tag{3}$$

which suggests a method for calculating arctan$x$; this also seems to come 'out of the blue' and we indicate some clue to it below.

The tangent function is an odd function of its argument whose leading term in a Taylor series expansion is linear. Hence we may write equation (3), after cancellation of the leading negative power of 2, as

$$a_i = \frac{x}{\theta}\left[1 + A_2\left(2^{-i}\theta\right)^2 + A_4\left(2^{-i}\theta\right)^4 + \ldots\right] \tag{4}$$

where A_2, A_4 ... are coefficients that we can eliminate without explicitly knowing what they are to accelerate the computation. We eliminate the term in θ^2 from the pairs (a_0, a_1), (a_1, a_2), ... giving γ_0, γ_1, ..., say. We have

$$a_0 = \frac{x}{\theta}\left(1 + A_2\theta^2 + A_4\theta^4 + \ldots\right), \tag{5}$$

and

$$a_1 = \frac{x}{\theta}\left[1 + A_2\left(\frac{\theta}{2}\right)^2 + A_4\left(\frac{\theta}{2}\right)^4 + \ldots\right]. \tag{6}$$

We multiply equation (6) by 4 and subtract equation (5) to remove the term in θ^2 and find

$$\gamma_0 = \frac{4a_1 - a_0}{3} = \frac{x}{\theta}\left(1 + B_4\theta^4 + B_6\theta^6 + \ldots\right) \tag{7}$$

where B_4, B_6 ... are coefficients (depending on A_4, A_6 ...) that we do not need to know explicitly because we shall eliminate them. We remove the negative sign on the right hand side of equation (7) with the aid of equation (1) to remove possible cancellation errors; we obtain

$$\gamma_0 = \frac{a_0 + 2b_0}{3} = \frac{x}{\theta}\left(1 + B_4\theta^4 + B_6\theta^6 + \ldots\right). \tag{8}$$

Similarly we find

$$\gamma_1 = \frac{a_1 + 2b_1}{3} = \left[1 + B_4\left(\frac{\theta}{2}\right)^4 + B_6\left(\frac{\theta}{2}\right)^6 + \ldots\right]. \tag{9}$$

We multiply equation (9) by 16 and subtract equation (8) to remove the term in θ^4 and then we use equation (1) to remove any negative signs. Continuing to eliminate terms in higher and higher powers of θ we find after tedious but straightforward algebra that, to a very good approximation,

$$S = \frac{x}{\theta} \tag{10}$$

where

$$S = a_0V_0 + b_0V_1 + b_1V_2 + \ldots \tag{11}$$

in which V_i are numbers to be determined. Thus

$$\theta = \arctan x = \frac{x}{S}. \tag{12}$$

The KDF9 algorithm uses the first 6 values of V_i; they are shown in Table 1. The value of a_0 is 1.

The algorithm is efficient. The errors for x chosen arbitrarily as 0.5, 1.0, 1.5 and 1000.0 are all smaller than $\frac{1}{4} \times 10^{-12}$.

Motivation for the sequences

We consider algebraic expressions involving the arctangent function. One of the simplest is the integral, in elementary calculus,

$$\int_a^\infty \frac{\mathrm{d}y}{1+y^2} = \arctan\left(\frac{1}{a}\right). \tag{13}$$

In any search for a series representation of the arctangent function it is advantageous to make the argument small. We can achieve this by generalising the integral by introducing a positive parameter c, say, to reduce the argument of the right hand side; we also allow a (assumed positive) to vary in such a way that the integral is invariant when c is changed. The generalised integral is

$$I(a,c) = \int_a^\infty \frac{\mathrm{d}y}{c^2+y^2} = \frac{1}{c}\arctan\left(\frac{c}{a}\right); \tag{14}$$

the utility of invariance is suggested by its simple form when $c = 0$. We reduce the argument by replacing c by $\frac{c}{2}$ and replace a by α, say, to ensure that I does not change; we require that

$$I(a,c) = I\left(\alpha, \frac{c}{2}\right) \tag{15}$$

which, from c times equation (14), is equivalent to requiring that

$$\arctan\left(\frac{c}{a}\right) = 2 \times \arctan\left(\frac{c}{2\alpha}\right). \tag{16}$$

Taking the tangent of both sides of equation (16) and using the formula $\tan(2\phi) = 2\tan\phi/(1-\tan^2\phi)$, we find that α satsfies the quadratic equation

$$\frac{c}{a} = \frac{c}{\alpha} \times \frac{1}{1-\frac{c^2}{4\alpha^2}} \tag{17}$$

which has positive root

$$\alpha = \frac{a+\sqrt{a^2+c^2}}{2}. \tag{18}$$

Coercing a and α to be positive forces α to exceed a and hence ensures that replacing c by $\frac{c}{2}$ does indeed reduce the argument of the arctangent function.

The algebra is slightly simplified by introducing a parameter dependent on a and c

$$b = \sqrt{a^2+c^2}, \tag{19}$$

and its equivalent

$$\beta = \sqrt{\alpha^2 + c^2/4} \tag{20}$$

and regarding the integral (14) as being dependent on a and b rather than on a and c. Equation (18) becomes

$$\alpha = \frac{a+b}{2}. \tag{21}$$

and, from equations (18), (19) and (20) we find

$$\beta = \sqrt{\alpha b}. \tag{22}$$

Thus equation (15) is equivalent to

$$I(a,b) = I(\alpha, \beta) \tag{23}$$

where α is the arithmetic mean of a and b and β is the geometric mean of α and b. There is nothing in these derivations that requires only one reduction of the argument of the arctangent function. We can generate sequences starting from a and b; comparing equations (1), (2), (21) and (22) we see that these are generated exactly as are the sequences $\{a_i\}$ and $\{b_i\}$ above. We can also generate a sequence $\{c_i\}$ starting with c where

$$c_i = 2^{-i}c = 2^{-i}c_0. \tag{24}$$

With $a_0 = 1$ and $b_0 = \sqrt{1+x^2}$ ($c_0 = x$) we find, from equations (14), (15) and (24)

$$\frac{1}{x}\mathrm{arctan} x = \frac{2^i}{x}\mathrm{arctan}\left(\frac{2^{-i}x}{a_i}\right) \tag{25}$$

which leads to equation (3).

Discussions of series generated by various arithmetic and geometric means, of transformations that leave certain integrals invariant and of calculations of π (closely related to calculations of the arctangent function) are given in references [1], [2] and [3].

Table 1: Coefficients $V_i = N_i/D_i$

i	Numerator N_i	Denominator D_i	V_i
0	28165298	1479104550	0.019042127887
1	28165300	1479104550	0.019042129240
2	56327872	1479104550	0.038082414120
3	113397760	1479104550	0.076666493927
4	179306496	1479104550	0.121226383896
5	1073741824	1479104550	0.725940450930

References

[1] Carlson B. C., 1971, *American Mathematical Monthly*, **78**, 496-505.

[2] Carlson B. C., 1972, *Mathematics of Computation*, **26**, 543-549.

[3] Salamin E., 1976, *Mathematics of Computation*, **30**, 565-570.